SFB 1078

Protonation Dynamics in Protein Function

Colloquium

Mon, **Dec. 8,** 2014

16:15 – 18:30

Freie Universität Berlin
Physics Department
Lecture Hall A

(Arnimallee 14, 14195 Berlin-Dahlem)

Invited speakers

Prof. Sebastian Westenhoff – University of Gothenburg – Sweden

Signal amplification and transduction in phytochrome photosensors disclosed by time-resolved X-ray scattering

Dr. Westenhoff will discuss recent findings on the structural dynamics of signal transduction in bacterial phytochromes. He will present crystal and solution structures showing an open and closed form of the dimeric protein for the activated and resting states, respectively. This nanometer-scale rearrangement is controlled by refolding of an evolutionarily conserved 'arm', which is in contact with the chromophore. These conclusions are drawn by combining protein crystallography, time-resolved X-ray solution scattering and molecular dynamics simulations. Dr. Westenhoff will discuss this new approach to protein structural dynamics. It opens up for studying the structural dynamics of protein complexes in real time and in solution. (Full abstract is available online.)

Prof. Johannes Neugebauer – Westfälische Wilhelms-Universität Münster

Beyond QM/MM: Quantum Chemical Methods for Spectroscopy, Energy-, and Electron-Transfer in Proteins

In his talk, Prof. Neugebauer will present recent developments for focused QM/QM methods suited to describe excited electronic states, excitation-energy-transfer, and electron-transfer couplings in large (bio-)chemical systems. Strategies to use this methodolgy for entire proteins will be discussed. Furthermore, selective QM algorithms suited for calculations of vibrational and vibronic spectral features of protein cofactors will be presented.

Coffee and tea are ready at 16:00 and during the break from 17:10 – 17:30. *www.sfb1078.de*

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